

1 **Revision 1**

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3 **Hydroxymcglassonite-(K),  $\text{KSr}_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ , the first Sr-bearing**  
4 **member of the apophyllite group, from the Wessels mine,**  
5 **Kalahari Manganese Field, South Africa**

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15  
16 **Abstract**

17 A new mineral species, hydroxymcglassonite-(K), ideally  $\text{KSr}_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ ,  
18 has been found in the Wessels mine, Kalahari Manganese Field, Northern Cape Province,  
19 South Africa. It is granular (<0.05 mm), associated with meieranite, sugilite, aegirine,  
20 pectolite, and yuzuxiangite. The mineral is colorless, transparent with white streak and  
21 vitreous luster. It is brittle and has a Mohs hardness of 4.5-5.0; cleavage is perfect on  
22 {001} and no parting or twinning was observed. The measured and calculated densities  
23 are 2.60(3) and 2.614 g/cm<sup>3</sup>, respectively. Optically, hydroxymcglassonite-(K) is uniaxial  
24 (+), with  $\omega = 1.555(5)$ ,  $\varepsilon = 1.567(5)$  (white light), and absorption  $O > E$ .

25 Hydroxymcglassonite-(K) is insoluble in water or hydrochloric acid. An electron  
26 microprobe analysis yielded an empirical formula (based on 13 non-H cations *pfu*)  
27  $\text{K}_{1.01}(\text{Sr}_{2.99}\text{Ca}_{1.03})_{\Sigma 4.02}\text{Si}_{7.99}\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ , which can be simplified to  
28  $\text{K}(\text{Sr},\text{Ca})_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ .

29 Hydroxymcglassonite-(K) is tetragonal with space group *P4/mnc* and unit-cell  
30 parameters  $a = 9.0792(2)$ ,  $c = 16.1551(9)$  Å,  $V = 1331.70(9)$  Å<sup>3</sup>, and  $Z = 2$ . It is  
31 isostructural with hydroxyapophyllite-(K),  $\text{KCa}_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ , with Sr substituting  
32 for Ca. The crystal structure of hydroxymcglassonite-(K) is characterized by  $\text{SiO}_4$

33 tetrahedra sharing corners to form  $(\text{Si}_8\text{O}_{20})^{8-}$  sheets parallel to (001), which are connected  
34 by the K and B (= Sr + Ca) cations, as well as hydrogen bonding. The K cation is  
35 coordinated by eight  $\text{H}_2\text{O}$  groups and the average K–O distance of 2.941(3) Å is shorter  
36 than that of 2.950(3) – 2.975(3) Å in hydroxyapophyllite-(K) or fluorapophyllite-(K). The  
37 B cation is 7-coordinated (4O + 2 $\text{H}_2\text{O}$  + OH) and the average B–O distance of 2.522 (3)  
38 Å is noticeably longer than that of 2.422 – 2.435 Å in hydroxyapophyllite-(K) or  
39 fluorapophyllite-(K). The Raman spectra of hydroxymcglassonite-(K) and  
40 hydroxyapophyllite-(K) are very comparable, especially in the O-H stretching region.  
41 The discovery of hydroxymcglassonite-(K), the first Sr-bearing mineral of the apophyllite  
42 group, implies that more Sr-bearing members of the group may be found in nature or  
43 synthesized in laboratories, but the possibility for an incomplete solid solution between  
44 hydroxyapophyllite-(K) and hydroxymcglassonite-(K), due to the size difference between  
45  $\text{Sr}^{2+}$  and  $\text{Ca}^{2+}$ , cannot be ruled out.

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47 **Key words:** hydroxymcglassonite-(K), apophyllite, new mineral, crystal structure, X-ray  
48 diffraction, Raman spectra

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## Introduction

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A new mineral species, hydroxymcglassonite-(K), ideally  $\text{KSr}_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$ ,  
has been found in the Wessels mine, Kalahari Manganese Fields, Northern Cape  
Province, Republic of South Africa. It is named in honor of Mr. James (Jim) A.  
McGlasson, who has been interested in collecting minerals since age 10, and started field  
collecting after graduation from college. Jim earned his B.S. degree in geology at the  
New Mexico Institute of Mining and Technology and M.S. degree in geology at the  
Colorado School of Mines. A successful 45-year career as an exploration geologist, mine  
manager, and consultant has allowed him to obtain geological and mineralogical  
knowledge at many diverse deposits worldwide. Jim has served as the president of the

60 Tucson Gem and Mineral Society, and on the board of directors of the Friends of  
61 Mineralogy. With a strong belief that getting children interested in science of any kind,  
62 especially geology and mineralogy, is critical for our society and future, he has been  
63 actively and constantly involved in various educational programs for children and young  
64 students, and has donated considerable amounts of mineral specimens for their  
65 interests/hobbies. Since his retirement in 2016, Jim has been a volunteer at the University  
66 of Arizona Mineral Museum and the mineralogy laboratory of the Department of  
67 Geosciences at the University of Arizona to continue his passion for minerals while  
68 contributing his knowledge and experience to help the society and other people. The new  
69 mineral and its name have been approved by the Commission on New Minerals,  
70 Nomenclature and Classification (CNMNC) of the International Mineralogical  
71 Association (IMA 2020-066). The cotype samples have been deposited at the University  
72 of Arizona Mineral Museum (Catalogue # 22691) and the RRUFF Project (deposition #  
73 R200004), which is a part of the University of Arizona Mineral Museum.

74 Hydroxymcglassonite-(K) is the first Sr-bearing mineral of the apophyllite group.  
75 This paper describes its physical and chemical properties and its crystal structure  
76 determined from single-crystal X-ray diffraction data.

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## 78 **Sample Description and Experimental Methods**

### 79 *Occurrence, physical and chemical properties, and Raman spectra*

80 Hydroxymcglassonite-(K) was found on a specimen (**Fig. 1**) collected from the  
81 Wessels mine, Kalahari Manganese Field, Northern Cape Province, Republic of South  
82 Africa (27° 6'51.82"S, 22°51'18.31"E). This specimen is also the type sample for  
83 meieranite (Yang et al. 2019) and yuzuxiangite (Gu et al. 2021). Hydroxymcglassonite-  
84 (K) crystals are found intergrown with isolated blue granular meieranite aggregates,  
85 which are embedded in a matrix consisting of mainly massive pale-green sugilite, along  
86 with minor prismatic grey aegirine, bladed white pectolite, and fibrous brownish

87 yuzuxiangite (Figs 2, 3, and 4). The mineral assemblage probably formed as a result of a  
88 hydrothermal event. Conditions during metamorphism were in the range of 270-420 °C at  
89 0.2-1.0 kbar (Kleyenstuber 1984; Gutzmer and Beukes 1996). Detailed reviews on the  
90 geology and mineralogy of the Kalahari Manganese Field have been presented by  
91 Kleyenstuber (1984), Von Bezings *et al.* (1991), and Gutzmer & Beukes (1996).

92 Hydroxymcglassonite-(K) crystals are granular (< 0.05 mm). The mineral is  
93 colorless, transparent with white streak and vitreous luster. It is brittle and has a Mohs  
94 hardness of 4.5-5.0; cleavage is perfect on {010} and no twinning was observed. The  
95 density measured floatation in heavy in liquids is 2.60(3) g/cm<sup>3</sup> and the calculated density  
96 is 2.614 g/cm<sup>3</sup>. Optically, hydroxymcglassonite-(K) is uniaxial (+), with  $\omega = 1.555(5)$ ,  $\epsilon$   
97 = 1.567(5) (white light), and absorption  $O > E$ . The compatibility index based on the  
98 empirical formula is 0.031 (excellent) (Mandarino 1981). Hydroxymcglassonite-(K) is  
99 insoluble in water or hydrochloric acid.

100 The chemical composition of hydroxymcglassonite-(K) was determined using a  
101 Shimadzu EPMA-1720 electron microprobe (WDS mode, 15 kV, 10 nA, and a beam  
102 diameter of 5  $\mu$ m). Because of the small size and vulnerability to the damage  
103 (dehydration) by the electron beam, only 5 analysis points were obtained from the single  
104 crystal used for the X-ray structure determination. As minerals in the apophyllite group  
105 commonly have the OH-F substitution, before the measurements, fluorine was  
106 particularly searched by the EDS method and then checked by the WDS scan for the  $F_{K\alpha}$   
107 peak. No F was detected by either methods with a detection limit of ~0.08 wt%. The  
108 standards used are listed in Table 1, along with the determined compositions. The  
109 resultant chemical formula, calculated on the basis of 13 non-H cations *pfu*, is  
110  $K_{1.01}(Sr_{2.99}Ca_{1.03})_{\Sigma 4.02}Si_{7.99}O_{20}(OH) \cdot 8H_2O$ , which can be simplified to  
111  $K(Sr,Ca)_4Si_8O_{20}(OH) \cdot 8H_2O$ . It should be pointed out that the Sr and Ca contents vary  
112 noticeably from point to point and are inversely correlated, resulting in the large standard  
113 deviations in their measurements. The crystal analyzed has Sr/(Sr+Ca)=75%. We also

114 found another crystal with  $\text{Sr}/(\text{Sr}+\text{Ca}) > 80\%$ , but its structure data are not as good as  
115 those reported here.

116 The Raman spectrum of hydroxymcglassonite-(K) was collected from a randomly  
117 oriented crystal on a Horiba Labram HR spectrometer in the State Key Laboratory of  
118 Powder Metallurgy, Central South University, China. The laser beam (488 nm, laser  
119 power 2 mW) was focused to 1  $\mu\text{m}$  with a 100 $\times$  objective on an Olympus  
120 microscope. The time of each scan in the range 100-4000  $\text{cm}^{-1}$  was 20 minutes with a  
121 resolution of 2  $\text{cm}^{-1}$ .

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### 123 *X-ray crystallography*

124 The powder X-ray diffraction data for hydroxymcglassonite-(K) were collected on  
125 a Rigaku Xtalab Synergy single crystal diffractometer ( $\text{MoK}\alpha$  radiation) in powder mode  
126 at 50KV and 1mA (Table 2, deposited). The unit-cell parameters obtained from the  
127 powder X-ray diffraction data using the program by Holland and Redfern (1997) are:  $a =$   
128 9.0928 (6),  $c = 16.203$  (2)  $\text{\AA}$ , and  $V = 1339.65$ (4)  $\text{\AA}^3$ .

129 Single-crystal X-ray diffraction data for hydroxymcglassonite-(K) were collected  
130 from a 0.010 x 0.002 x 0.002 mm crystal on a Rigaku Xtalab Synerg D/S 4-circle  
131 diffractometer equipped with  $\text{MoK}\alpha$  radiation. All reflections were indexed on the basis  
132 of a tetragonal unit-cell (Table 3). The systematic absences of reflections are compatible  
133 with space groups  $P4nc$  (#104) and  $P4/mnc$  (#128). The crystal structure was solved and  
134 refined using SHELX-2018 (Sheldrick 2015a, 2015b) based on space group  $P4/mnc$ ,  
135 because it produced the better refinement statistics in terms of bond lengths and angles,  
136 atomic displacement parameters, and  $R$  factors. Difference Fourier syntheses only  
137 revealed the two H atoms (H1 and H2) associated with the  $\text{H}_2\text{O}$  group (O4), but failed to  
138 locate the H atom in the OH group (O5). This is not surprising, considering that there are  
139 only two equivalent H atoms from the OH group per unit-cell, but 16 equivalent ones for  
140 each H1 and H2. During the refinements, the structure chemistry was constrained to the

141 empirical formula determined from the electron microprobe analysis, i.e.,  
142  $K_{1.00}(Sr_{2.98}Ca_{1.02})_{\Sigma=4.00}Si_8O_{20}(OH)\cdot 8H_2O$ . All non-H atoms were refined anisotropically,  
143 whereas the two H atoms (H1 and H2) were refined isotropically. Final atomic  
144 coordinates and displacement parameters for hydroxymcglassonite-(K) are given in  
145 [Tables 4 and 5](#), respectively. Selected bond distances are presented in [Table 6](#).

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### 147 **Crystal structure description and discussion**

148 Hydroxymcglassonite-(K), ideally  $KSr_4Si_8O_{20}(OH)\cdot 8H_2O$ , is isostructural with  
149 hydroxyapophyllite-(K),  $KCa_4Si_8O_{20}(OH)\cdot 8H_2O$  (Rouse et al. 1978) ([Table 3](#)), with Sr  
150 substituting for Ca. Its structure is characterized by  $SiO_4$  tetrahedra sharing corners to  
151 form  $(Si_8O_{20})^{8-}$  sheets parallel to (001) ([Fig. 5](#)), which are connected by the interstitial  $K^+$   
152 and  $B^{2+}$  (=Sr + Ca) cations and by hydrogen bonding. In the sheet,  $SiO_4$  tetrahedra form  
153 4- and 8-membered rings ([Fig. 5](#)). The geometry of hydrogen bonding is in accord with  
154 that in hydroxyapophyllite-(K) (Rouse et al. 1978). The bond-valence sums calculated  
155 using the parameters from Brese and O'Keeffe (1991) ([Table 7](#)) indicate that O4 is  $H_2O$   
156 and O5 is OH.

157 The  $K^+$  cation in hydroxymcglassonite-(K) is coordinated by eight  $H_2O$  groups.  
158 The average K–O distance of 2.941(3) Å ([Table 6](#)) is shorter than that of 2.950(3) –  
159 2.975(3) Å in hydroxyapophyllite-(K) (Rouse et al. 1978) or fluorapophyllite-(K) (Chao  
160 1971; Colville et al. 1971; Prince 1971; Pechar 1987; Ståhl et al. 1987). The  $B$  (= 0.74Sr  
161 + 0.26Ca) cation is 7-coordinated (4O + 2 $H_2O$  + OH). The average  $B$ –O distance of  
162 2.522 (3) Å in hydroxymcglassonite-(K) ([Table 6](#)) is noticeably longer than that of 2.422  
163 – 2.435 Å in hydroxyapophyllite-(K) (Rouse et al. 1978) or fluorapophyllite-(K) (Chao  
164 1971; Colville et al. 1971; Prince 1971; Pechar 1987; Ståhl et al. 1987). This is  
165 understandable, as the  $B$  site is predominantly occupied by  $Ca^{2+}$  in both  
166 hydroxyapophyllite-(K) and fluorapophyllite-(K), which is significantly smaller than  $Sr^{2+}$   
167 in ionic radius (1.06 vs. 1.21 Å) (Shannon 1976).

168 In the ruizite-strontioruizite solid solution  $(\text{Ca,Sr})_2\text{Mn}^{3+}_2\text{Si}_4\text{O}_{11}(\text{OH})_4 \cdot 2\text{H}_2\text{O}$ , the  $B$   
169 cation ( $B = \text{Ca} + \text{Sr}$ ) is also 7-coordinated (Hawthorne, 1984; Fendrich et al. 2016; Yang  
170 et al. 2021) and the average  $B$ -O bond distance increases linearly with increasing  $X =$   
171  $\text{Sr}/(\text{Sr} + \text{Ca})$ , following the equation  $\langle B\text{-O} \rangle = 0.1468X + 2.4475$  (Å) ( $R^2 = 0.98$ ) (Yang et  
172 al. 2021). With  $\text{Sr} = 0.74$  for hydroxymcglassonite-(K), we obtain  $\langle B\text{-O} \rangle = 2.556$  Å,  
173 which is slightly longer than our measured value of 2.522 Å.

174 The Raman spectrum of hydroxymcglassonite-(K) is plotted in **Figure 6**. Based on  
175 previous Raman spectroscopic studies on both hydroxyapophyllite-(K) and  
176 fluorapophyllite-(K) (Adams et al. 1980; Sidorov 2000; Frost and Xi 2012; Goryainov et  
177 al. 2012; Ogorodova et al. 2019), we made the tentative assignments of major Raman  
178 bands for hydroxymcglassonite-(K) (**Table 8**). For comparison, the Raman spectra of  
179 hydroxyapophyllite-(K) (<http://rruff.info/R050169>) and fluorapophyllite-(K)  
180 (<http://rruff.info/R050021>) from the RRUFF Project were also plotted in **Figure 6**. The  
181 similarities among the three spectra are evident. The difference in peak intensities among  
182 the spectra principally results from the different crystal orientations when the data were  
183 collected.

184 According to Frost and Xi (2012), Goryainov et al. (2012), and Ogorodova et al.  
185 (2019), the key difference between the Raman spectra of hydroxyapophyllite-(K) and  
186 fluorapophyllite-(K) is the observation of two Raman bands in the O-H stretching region  
187 at  $\sim 3565$  (due to the O-H stretching vibrations in  $\text{H}_2\text{O}$ ) and  $3625 \text{ cm}^{-1}$  (due to the O-H  
188 stretching vibrations in OH) for the former and only one band at  $\sim 3565 \text{ cm}^{-1}$  for the latter.  
189 The observation of the Raman peak at  $\sim 3625 \text{ cm}^{-1}$  is regarded as a distinctive diagnostic  
190 feature indicating the presence of the OH group in the apophyllite-type structures  
191 (Ogorodova et al. 2019). The Raman spectrum of hydroxymcglassonite-(K) exhibits two  
192 major bands in the O-H stretching vibration region, consistent with that of  
193 hydroxyapophyllite-(K), indicating the presence of both  $\text{H}_2\text{O}$  and OH groups in its  
194 structure.

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## Implications

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Apophyllite-type minerals are of great industrial and technological interest

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because they are examples of naturally occurring single-sheet silicates and their reactions

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with chlorosilanes yield apophyllite-based organosilicate polymers on both sides of

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silicate sheets, which possess a unique combination of hydrophobic and hydrophilic

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properties that are highly tunable (Chao et al., 2001; Chen et al., 2007; Specht et al.,

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2010). According to the IMA-CNMNC guidelines for mineral nomenclature (Hatert et al.

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2013), minerals of the apophyllite group are named based on the chemical formula

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$A^+Ca_4Si_8O_{20}X \cdot 8H_2O$ , where  $A^+$  (= K, Na, Cs, or  $NH_4$ ) and  $X$  (= F or OH) are used as

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suffixes and prefixes (fluor for F and hydroxy for OH), respectively, in the naming. To

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date, there are five members in the apophyllite group: fluorapophyllite-(K),

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fluorapophyllite-(Na), fluorapophyllite-( $NH_4$ ), fluorapophyllite-(Cs), and

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hydroxyapophyllite-(K). The discovery of hydroxymcglassonite-(K), the first Sr-bearing

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member of the apophyllite group, suggests that more Sr-dominant members of the group

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may be found in nature or synthesized in laboratories. For naturally occurring Sr-

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dominant members, the same naming guidelines with  $A$  and  $X$  as suffixes and prefixes,

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respectively, should be employed.

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The  $Sr^{2+}$ - $Ca^{2+}$  substitution in various minerals and materials has been a subject of

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numerous investigations owing to its effects on the properties of luminescent materials

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(e.g., Yu et al., 2012; Misevicius et al. 2019; Wang et al. 2020), bioactive glasses (e.g.,

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Martin et al. 2012; Pedone et al. 2021), and solid solutions (e.g., Gottschalk et al. 1998;

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Ellemann-Olesen and Malcherek 2005). In some cases, the  $Sr^{2+}$ - $Ca^{2+}$  substitution may

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result in incomplete solid solutions due to the difference in the  $Ca^{2+}$  and  $Sr^{2+}$  ionic radii ( $r$

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= 1.06 Å for 7-coordinated  $Ca^{2+}$  and 1.21 Å for  $Sr^{2+}$ ) (Shannon 1976). There are two

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kinds of incomplete solid solutions. One of them is that the two endmembers assume

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different structure symmetries, such as  $CaCO_3$  ( $R-3c$  calcite) vs.  $SrCO_3$  ( $Pm\bar{c}n$



222 strontianite) or  $\text{CaSO}_4$  (*Bmmb* anhydrite) vs.  $\text{SrSO}_4$  (*Pnma* celestine). The other kind is  
223 that the two endmembers possess the same symmetry, but it is different from that for the  
224 intermediate phases, as a consequence of the  $\text{Ca}^{2+}$  and  $\text{Sr}^{2+}$  ordering into different  
225 crystallographic sites. For example, in the system of  $\text{Ca}_2\text{Mn}^{3+}_2\text{Si}_4\text{O}_{11}(\text{OH})_4 \cdot 2\text{H}_2\text{O}$   
226 (ruizite) ---  $\text{Sr}_2\text{Mn}^{3+}_2\text{Si}_4\text{O}_{11}(\text{OH})_4 \cdot 2\text{H}_2\text{O}$  (strontioruizite), the two endmembers have the  
227 same *C2* symmetry, but the intermediate phase with the  $\text{Ca}:\text{Sr} \cong 1:1$ , ideally  
228  $\text{SrCaMn}^{3+}_2\text{Si}_4\text{O}_{11}(\text{OH})_4 \cdot 2\text{H}_2\text{O}$  (taniajacoite), exhibits the *C-1* symmetry due to the  
229 preferential occupation of  $\text{Sr}^{2+}$  and  $\text{Ca}^{2+}$  over two distinct, 7-coordinated sites (Yang et al.  
230 2021). Since both hydroxyapophyllite-(K),  $\text{KCa}_4\text{Si}_8\text{O}_{20}(\text{OH}) \cdot 8\text{H}_2\text{O}$ , and  
231 hydroxymcglassonite-(K),  $\text{KSr}_4\text{Si}_8\text{O}_{20}(\text{OH}) \cdot 8\text{H}_2\text{O}$ , have the same symmetry *P4/mnc*, it  
232 then begs the question whether the intermediate phase,  $\text{K}(\text{Sr}_2\text{Ca}_2)\text{Si}_8\text{O}_{20}(\text{OH}) \cdot 8\text{H}_2\text{O}$ ,  
233 possesses the same symmetry as the two endmembers. In other words, could  $\text{Sr}^{2+}$  and  
234  $\text{Ca}^{2+}$  in the intermediate phase be ordered into two distinct sites, as in taniajacoite, thus  
235 resulting in a reduction in the structure symmetry? Interestingly, Matsueda et al. (1981)  
236 reported that fluorapophyllite-(Na),  $\text{NaCa}_4\text{Si}_8\text{O}_{20}\text{F} \cdot 8\text{H}_2\text{O}$ , exhibits the orthorhombic  
237 symmetry *Pnmm*, rather than the tetragonal symmetry *P4/mnc* as for fluorapophyllite-(K).  
238 They ascribed this symmetry reduction to the silicate-sheet distortion caused by the  
239 substitution of small  $\text{Na}^+$  for large  $\text{K}^+$ . As a consequence, the 8-fold position (*8h* with the  
240 site symmetry *m*) occupied by  $\text{Ca}^{2+}$  in the *P4/mnc* structure splits into two 4-fold  
241 positions (*4g* with the site symmetry *m*), Ca1 and Ca2, in the *Pnmm* structure. An  
242 examination of the fluorapophyllite-(Na) structure (Matsueda et al. 1981) reveals that,  
243 although both Ca1 and Ca2 sites are still 7-coordinated, as in fluorapophyllite-(K), the  
244 Ca1 site is significantly larger than the Ca2 site, with  $\langle \text{Ca1}-(\text{O},\text{F}) \rangle = 2.426 \text{ \AA}$  vs.  $\langle \text{Ca2}-$   
245  $(\text{O},\text{F}) \rangle = 2.367 \text{ \AA}$ . This observation suggests that the apophyllite-type structure is  
246 intrinsically capable of assuming an ordered orthorhombic *Pnmm* structure with the Ca1  
247 and Ca2 sites occupied by two different  $B^{2+}$  cations. Thus, we cannot rule out the  
248 possibility that the intermediate phase between hydroxyapophyllite-(K) and

249 hydroxymcglassonite-(K) could possess an ordered structure with large  $\text{Sr}^{2+}$  and small  
250  $\text{Ca}^{2+}$  occupying two distinct sites, such as the Ca1 and Ca2 sites in fluorapophyllite-(Na)  
251 (Matsueda et al. 1981).

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256 Å. Koda.

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378 **List of Figure Captions**

- 379  
380 Figure 1. The specimen on which colorless hydroxymcglassonite-(K) crystals are found  
381 in intergrowth with isolated blue granular meieranite aggregates, which are embedded in  
382 a matrix consisting of mainly massive pale-green sugilite, along with minor prismatic  
383 grey aegirine, bladed white pectolite, and brownish fibrous yuzuxiangite.  
384  
385 Figure 2. A microscopic view of colorless hydroxymcglassonite-(K) intergrown with blue  
386 granular meieranite.  
387  
388 Figure 3. A photomicrograph showing the occurrence and association of  
389 hydroxymcglassonite-(K) (reflected light, parallel nicols).  
390  
391 Figure 4. Backscattered electron image of hydroxymcglassonite-(K), associated with  
392 meieranite and sugilite.  
393  
394 Figure 5. Raman spectra of hydroxymcglassonite-(K), hydroxyapophyllite-(K), and  
395 fluorapophyllite-(K).  
396  
397 Figure 6. Crystal structure of hydroxymcglassonite-(K). SiO<sub>4</sub> tetrahedra and Sr-dominant  
398 polyhedra are green and yellow, respectively. The K, O4 (H<sub>2</sub>O), O5 (OH), and H atoms  
399 are shown as large purple, medium aqua, medium red, and small blue spheres,  
400 respectively. Thin black lines show the unit cell.

403 **List of Tables**

- 404  
405 Table 1. Chemical composition of hydroxymcglassonite-(K).  
406  
407 Table 2. Powder X-ray diffraction data for hydroxymcglassonite-(K).  
408  
409 Table 3. Summary of crystallographic data and refinement results for  
410 hydroxymcglassonite-(K).  
411  
412 Table 4. Fractional atomic coordinates and isotropic or equivalent isotropic displacement  
413 parameters (Å<sup>2</sup>) for hydroxymcglassonite-(K).  
414  
415 Table 5. Atomic displacement parameters (Å<sup>2</sup>) for hydroxymcglassonite-(K).  
416  
417 Table 6. Selected bond distances (Å) in hydroxymcglassonite-(K).  
418  
419 Table 7. Bond-valence sums for hydroxymcglassonite-(K).  
420  
421 Table 8. Tentative assignments of major Raman bands for hydroxymcglassonite-(K).  
422

Table 1. Electron microprobe analysis data (in wt.%) for hydroxymcglassonite-(K).

Constituent	Mean	Range	Stand. Dev.	Probe Standard
SiO <sub>2</sub>	45.99	44.94-47.27	0.99	SiO <sub>2</sub>
K <sub>2</sub> O	4.56	4.17-5.93	0.32	KAlSi <sub>3</sub> O <sub>8</sub>
CaO	5.52	3.06-7.21	2.19	CaSiO <sub>3</sub>
SrO	29.66	26.36-33.67	3.11	SrSO <sub>4</sub>
H <sub>2</sub> O*	14.67			
Total	100.40	100.05-100.78	0.28	

Note: \*Calculated based on the structure.

Table 3. Comparison of mineralogical data for hydroxyapophyllite-(K) and Hydroxymcglassonite-(K)

	hydroxyapophyllite-(K)	Hydroxymcglassonite-(K)
Ideal chemical formula	$\text{KCa}_4\text{Si}_8\text{O}_{20}(\text{OH},\text{F})\cdot 8\text{H}_2\text{O}$	$\text{KSr}_4\text{Si}_8\text{O}_{20}(\text{OH})\cdot 8\text{H}_2\text{O}$
Crystal symmetry	Tetragonal	Tetragonal
Space group	<i>P4/mnc</i>	<i>P4/mnc</i>
<i>a</i> (Å)	8.979(4)	9.0792(2)
<i>c</i> (Å)	15.83(1)	16.1551(9)
<i>V</i> (Å <sup>3</sup> )	1276.253	1331.70(10)
<i>Z</i>	2	2
$\rho_{\text{obs}}, \rho_{\text{cal}}$ (g/cm <sup>3</sup> )	2.37, 2.36	2.59, 2.60
Optical properties	uniaxial (+)	uniaxial (+)
$\omega$	1.52	1.555
$\varepsilon$	1.53	1.567
$2\theta$ range for data collection	$\leq 54.77$	$\leq 67.31$
No. of reflections collected	1049	10474
No. of independent reflections	757	1262
No. of reflections with $I > 2\sigma(I)$	696	1046
No. of parameters refined		61
R(int)		0.039
Final $R_1, wR_2$ factors [ $I > 2\sigma(I)$ ]	0.035, 0.038	0.040, 0.088
Goodness-of-fit		1.069
Reference	Rouse et al. (1978)	This study



Table 6. Selected bond distances (Å) for hydroxymcglassonite-(K) and hydroxyapophyllite-(K).

	Hydroxymcglassonite-(K)	Hydroxyapophyllite-(K)
K—O4 × 8	2.941(3)	2.954(3)
<i>B</i> —O3 × 2	2.487(2)	2.403(2)
—O3 × 2	2.509(2)	2.416(2)
—O5	2.5497(5)	2.435(1)
—O4 × 2	2.555(3)	2.486(3)
Ave.	2.522	2.435
Si—O3	1.590(2)	1.584(3)
—O1	1.6185(11)	1.622(3)
—O2	1.629(2)	1.617(2)
—O2	1.636(2)	1.644(2)
Ave.	1.619	1.616

Table 7. Bond-valence sums for hydroxymcglassonite-(K).

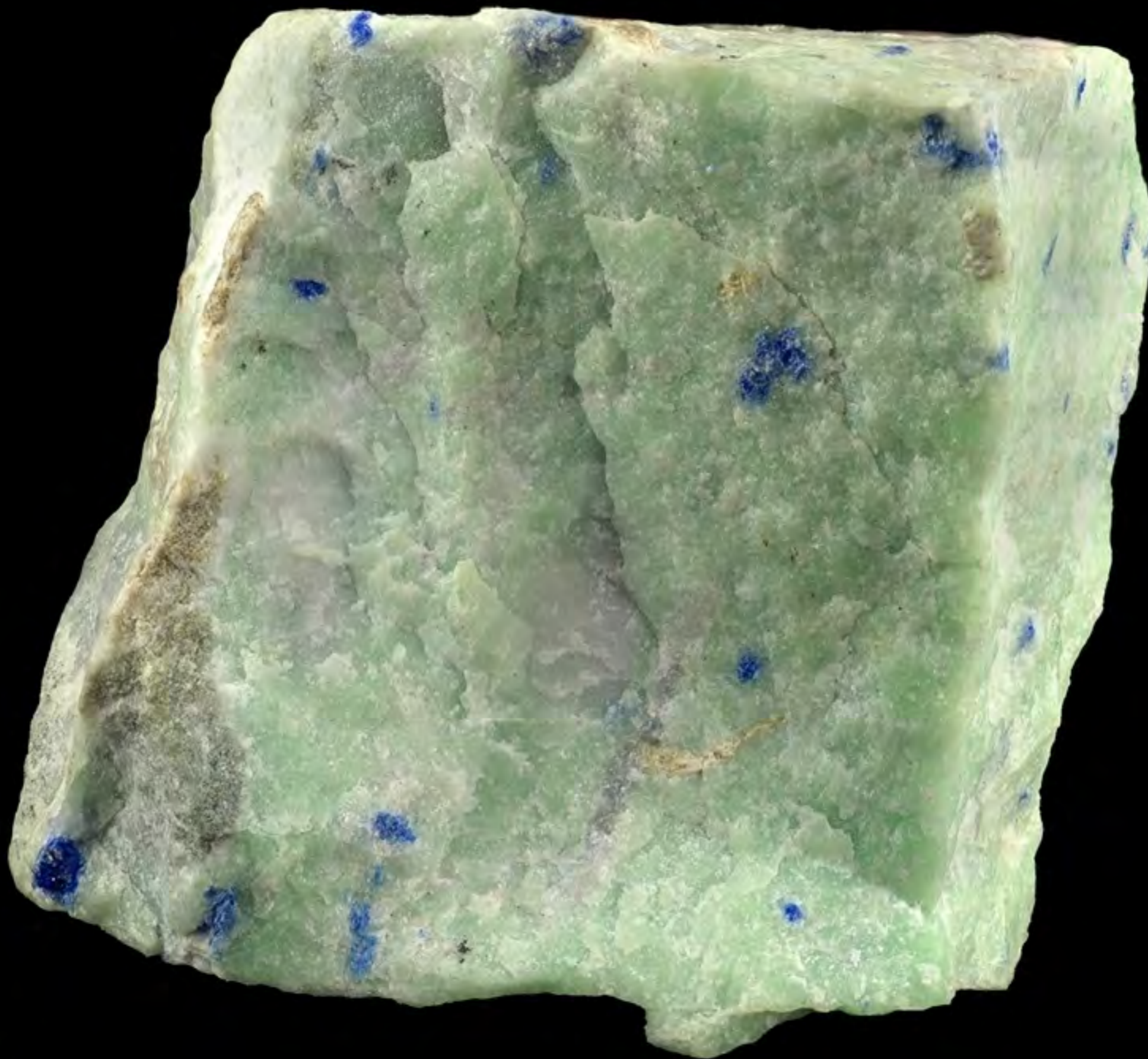
	K	B	Si	Sum
O1			1.015x2→	2.029
O2			0.984	1.953
			0.969	
O3		0.337 x2↓	1.100	1.754
		0.317 x2↓		
O4	0.112 x 8↓	0.280 x2↓		0.392
O5		0.237 x 4→		0.948
Sum	0.896	2.105	4.068	

Note: The bond valence sum for *B* was calculated based on  $(0.74\text{Sr}^{2+} + 0.26\text{Ca}^{2+})$ .

Table 8. Tentative assignments of major Raman bands for hydroxymcglassonite-(K).

Bands (cm <sup>-1</sup> )	Assignment
3621	O-H stretching vibration in OH groups
3572	O-H stretching vibration in H <sub>2</sub> O groups
940-1060	Si-O stretching vibrations in SiO <sub>4</sub> units
772, 861	H <sub>2</sub> O libration
662, 635	Si-O-Si bending vibrations
430, 574	O-Si-O bending vibrations
160-321	Lattice modes and <i>B</i> -O interaction vibrations

Note: *B* = Sr<sup>2+</sup> + Ca<sup>2+</sup>.

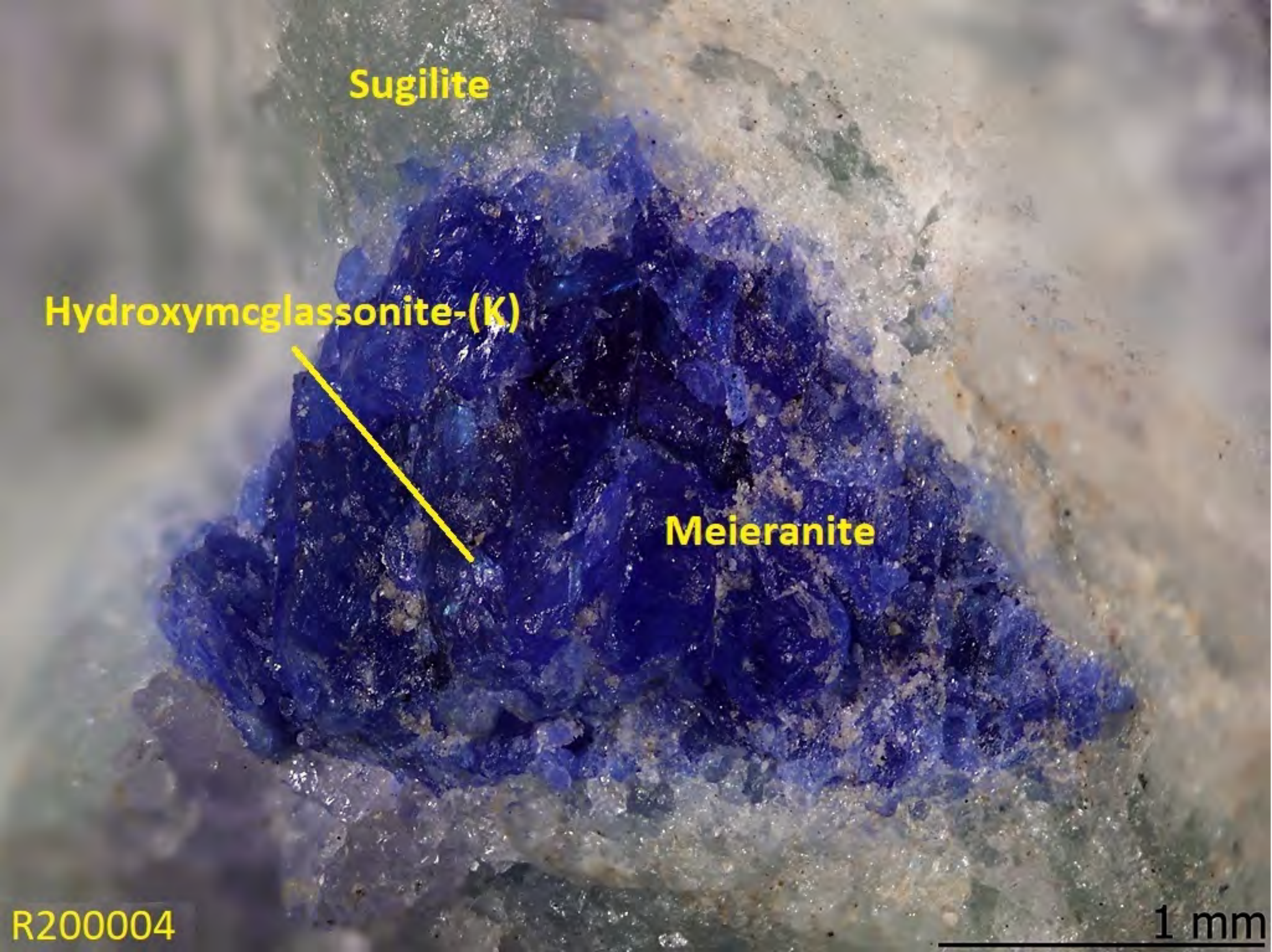


R200004

1 cm

Figure 1





Sugilite

Hydroxymcglassonite-(K)

Meieranite

1 mm

R200004

Figure 2.





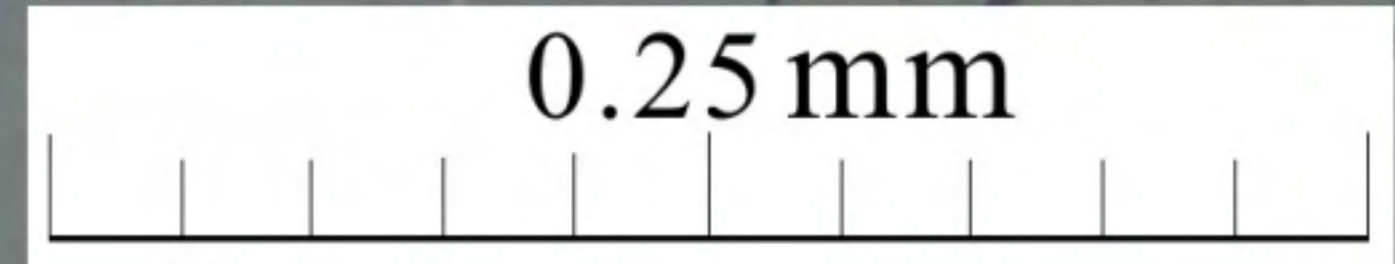
sugilite

Hydroxymcglassonite-(K)

meieranite

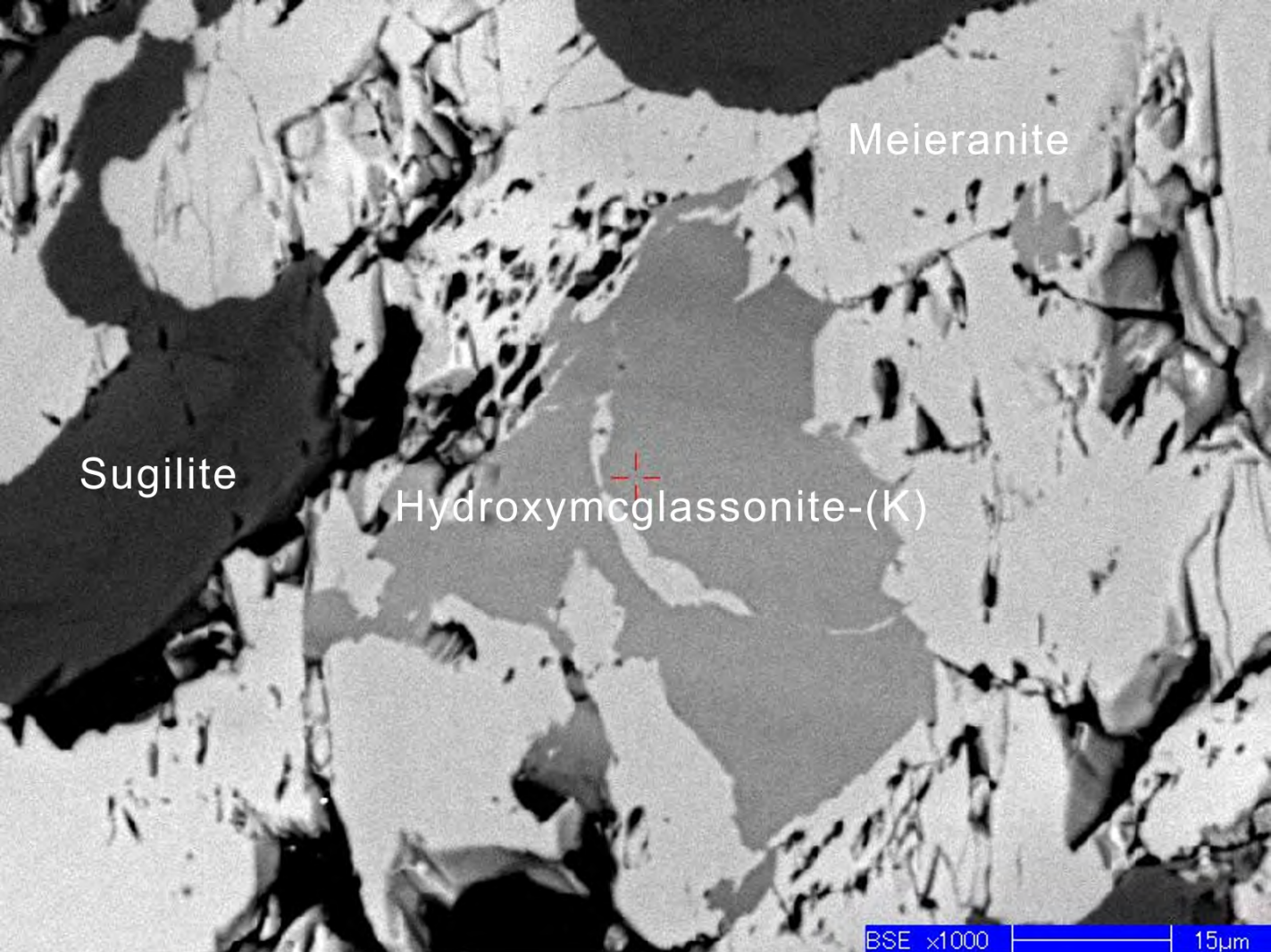
meieranite

sugilite



**Figure 3.**





**Figure 4.**

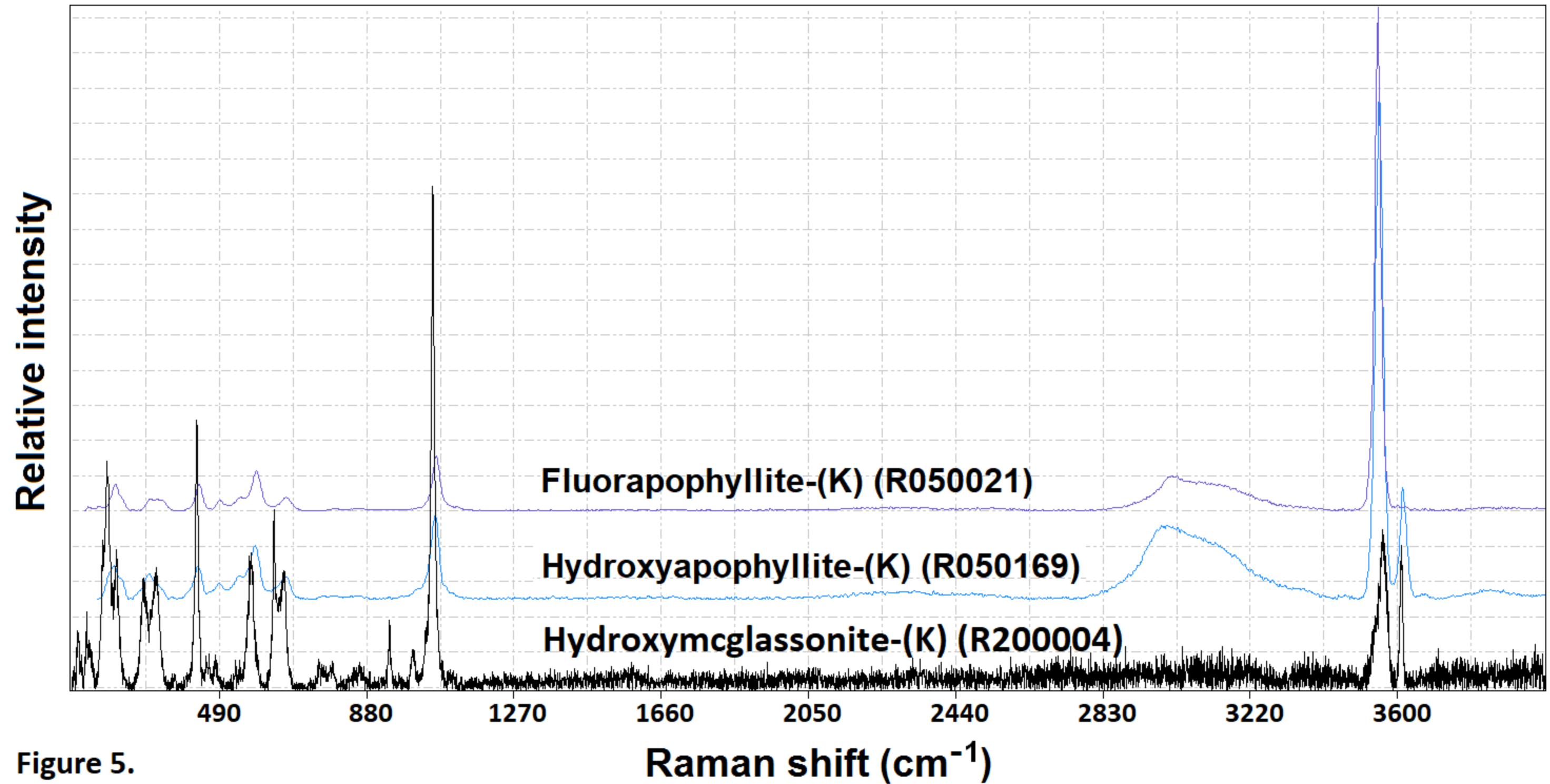


Figure 5.



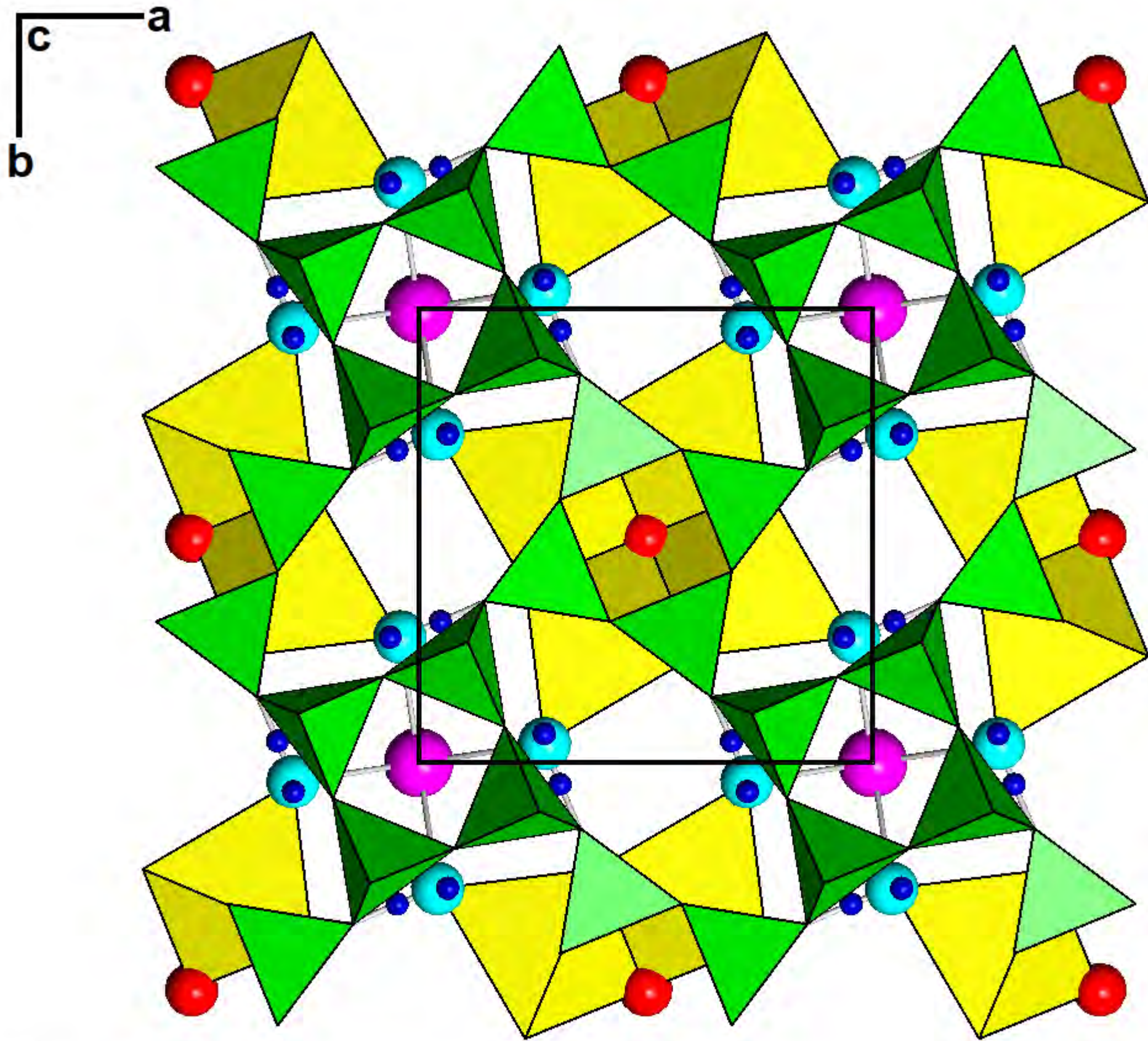


Figure 6.